1.0   Purpose

The purpose of this document is to provide a detailed coverage of the proposed modifications to the LANL Electronic Data Deliverable (EDD) which are currently being used to transmit analytic data from the contract laboratories to LANL. In reviewing the data we have received during the past eight months, it is apparent that there are a number of changes and clarifications which need to be made to the EDD in order for LANL to effectively use the data.

2.0   Perspective

Prior to the spring of 1995, analytic results from ER samples were provided by the contract laboratories only in hard copy format. Members of the CST data management team, reviewed the data, and then manually keyed it into their datatrieve database. The datatrieve data was then periodically transferred to FIMAD. In reviewing this process, the Environmental Restoration (ER) project expressed concern that the manual data entry process was error prone and inefficient. It was determined that a data necessary to perform electronic validation and verification were not being captured by the datatrieve system, and were thus not available in FIMAD.

In late 1994, the ER project determined that the best way to correct these issues and concerns would be to have the laboratories submit analytic results to LANL electronically and formed an electronic data working group to address the issues. Further, it was determined that existing electronic deliverables used by other laboratories and organizations to exchange information were not suitable for LANL's use and that a LANL specific EDD should be created.

The resulting LANL EDD is comprised of approximately 26 different file formats which can loosely be though of as spreadsheets (examples of these deliverables are included in Appendix B). Each deliverable contains the data which should be reported for a particular type of analysis. Data is generally submitted by the laboratories on a floppy disk, although some laboratories are able to transmit the data to LANL via the Internet. Analytic data has been reported by the contract laboratories using these formats since June 1995. During the past 8 months, the EDD has evolved several times as errors or omissions have been detected. Currently, the SMO has received more than 2,500 deliverables from both LANL and external contract laboratories. Additional deliverables are being received and processed by the SMO on a daily basis.

During summer and early fall of 1995, a variety of attempts were made to extract the analytic data from the various EDD formats which had been submitted from the laboratories and to insert them into a relational database so that the data could be accessed by the ER project. While some of these efforts were moderately successful, they were generally deemed to be incomplete and unacceptable.

In November of 1995, the job of reading the EDDs, validating the data and loading it into the database was given to FIMAD. Since that time, FIMAD has written the necessary code to extract the data from the various EDDs, perform rudimentary validation, and load the data into FIMAD's Oracle database. In the process of loading this data, FIMAD has determined that many of the fields of data are being used inconsistently by the laboratories. Other laboratories are not reporting data (such as the laboratory batch ID) which is vital to our use of the data.   The variability in laboratory reporting not only makes the task of loading data much more difficult, but it also has a significant impact on the ease with which ER personnel and regulators will be able to access and use the data received via the EDD.

While little can be done to readily fix the data which has already been received, these issues must be addressed in order to ensure that data we collect and process this field season will meet our needs. A significant portion of the variability in how the labs report the data can be traced directly to the poor (or in some cases missing) definition of the fields within each EDD. The purpose of this document, and the subsequent meeting with representatives of the analytical laboratories, is to provide a clear specification of how the data is to be reported as well as to provide an opportunity for review and comment.

2.1 Future Electronic Deliverables

In accordance with DOE orders, it is likely that LANL will adopt the DEEMS electronic data deliverable format within the next year. As such, our work with the current EDD should focus on providing more structure to the existing data fields which will enable LANL to effectively use the data currently being provided. Every effort should be made to avoid introducing new data fields into the current EDD or in making any changes which will cause significant hardships to the analytic laboratories.

3.0 Overview of Changes to the Current EDD

The proposed changes to the current EDD can be classified as: (1) deletion of fields which no longer need to be reported, (2) identification of required vs optional data, and (3) specification of the format and values to be reported in existing fields. No new fields of information have been added, nor does the structure of the existing EDD need to be significantly revised. Each of these is briefly described in the following sections.

3.1 Fields which are no longer reported

In reviewing the fields of data which we require the analytical laboratories to provide in the current EDD, it is apparent that a significant number of data fields are designed to support electronic validation of the analytic data. Unfortunately, we do not have all of the data necessary to perform these checks and it is unlikely that we will have the necessary data until we switch to the DEEMS deliverable. We should remove these fields from the current EDD.

In order to minimize the impact of this decision on the contract laboratories, labs may continue to report the data using the current EDD in its entirety. We will discard those fields which we have designated as being no longer reported. Optionally, the labs may use the existing EDD format leaving the associated data fields blank, or may simply not include the associated rows in their electronic exports.

3.2 Optional vs Required Fields

Some fields of data in the EDD must be provided in order to support our analysis, while others should be though of as optional. Fields which are designated as being "Required" must be supplied. EDDs which are missing required fields will be returned to the laboratory for correction. A field is "Optional" if a value is not required, but if provided will be captured and stored in FIMAD. For example, the "Time of Analysis" field is optional in all cases. Finally, a field may be "Optional" if a value is not always required -- for example, the second column result in some dual column methods is only required if a hit was detected in the first column.

Section 4 contains a detailed discussion of the fields that are required for the EDD in general. Appendix B contains copies of the individual EDDs. In both documents, each field is coded (in the type field) as being:

Type	Meaning	Description
R	Required	Data **must** be provided for this field.
O	Optional	Data may be provided for this field.
-	Not Necessary	Data is no longer requested. If provided, contents of this data field will be discarded.
*	data moved	Please see section 5.2 for more information

3.3   Specification of Format

Several key fields of data in the current EDD are loosely defined. A variety of different (and sometimes unexpected or unwanted) data is entered by the various contract laboratories. The data dictionary (section 4) provides a more rigorous definition of the contents of each field and the format in which the data should be reported. For example, a list of possible values for the "MATRIX" field includes: AIR, WATER, SOIL, SEDIMENTS, OIL, FILTER, and MISC. These are the only values which should be used to report normal (non QC) samples.

3.4   Summary of Changes

The following provides a summary of the proposed changes for each section of the EDD:

Section	Contents	Summary of Changes
A	Request	No significant changes are applied to this section.
B	Sample Header	All fields in this section must be provided. Data format specifications are now provided for key fields.
C	Analysis Header	The majority of fields in this section do not need to be reported. Data format specifications are now provided.
D	Comments	No significant changes are applied to this section.
E	Analytes	A number of fields have been deleted from this section. The analytes to be reported in each suite remain the same.
F	Carriers	No significant changes are applied to this section.
G	Tracers	Most fields of have been deleted from this section. Only the percent recovered needs to be reported.
H	Surrogates	The retention time is no longer required. Data sheets which erroneously specified "concentration" must be redefined so that the percent recovery for the surrogate is reported instead of the *amount* recovered. An '*' should be put in the LAB_QUALIFIER field for this record if the surrogate is out of control.
I	TICS	No significant changes are applied to this section.

4.0 Data Dictionary

Section 4 provides a detailed data dictionary for the modified EDD. In conjunction with the detailed EDDs appearing in appendix B, this section clearly defines each field in each EDD, and specifies whether values for the individual fields are required or not.

The data dictionary also provides information concerning the format of the data. The format column contains one or more of the following symbols:

Format	Description
#	a pound symbol (#) indicates a digit. For example, a field with a format of ### indicates that a maximum of three digits may be reported. Unless instructed to do so, you are not required to left pad with zeros.
Number	any valid number (i.e., an integer or floating point number). For floating point numbers, the number of digits of precision which should be reported is left up to the contract laboratory.
A###	An alpha numeric field with a maximum of ### digits. For example, a field with a format of A28 indicates that a maximum of 28 alphanumeric characters may be reported in this field.
Y or N	A single character of either 'Y' or 'N' should be reported in this field.
DD-MON-YY	All dates in the EDD are reported in this format. DD specifies the day of the month, MON a three character abbreviation for the month, and YY the last two digits of the year. For example, 23-JAN-96.
HH:MI	All times in the EDD are reported in this format. HH specifies the hour in 24 hour format, and MM specifies the minute. For example, 18:30.
N/A	No data needs to be reported in this field. Generally this format is associated with place holder fields.

4.1 Section A - Request Header

The Request Header section contains information which is the same for all samples which are part of a LANL sample delivery group. This section is identical for all EDD sheets. Data in section A should be repeated for each column of the EDD where you are reporting results. The data field names, their format and a brief description are shown in figure 1.

Tag	Label	type	Format	Description
A001	request header	-		
A002	version	R	#.#.#	Version number of the EDD. For this EDD it should be 0.0.4
A003	date of version release	-		Date of the EDD revision.
A004	LANL request number	R	#####	Identifies the delivery group sent out by LANL. Enter exactly as it appears on the LANL Service Agreement.
A005	laboratory	R	see listing	Abbreviated laboratory identifier.
A006	contract number	-		
A007	date of sample receipt by lab	R	DD-MON-YY (15-JAN-96)	Date when the sample was received by the contract laboratory..
A008	date of data submission to LANL	R	DD-MON-YY (15-JAN-96)	Date when results were sent to LANL (either in electronic or physical form).

Figure 1 - Definition for Section A

4.2   Section B - Sample Header

Section B contains the information which is specific to an individual sample. The Sample Header section is identical for all EDD sheets. Data in section B must be present for each column of the EDD where you are reporting results.

The data field names, their format and a brief description are shown in figure 2.

Tag	Label	type	Format	Description
B001	sample header	-		
B002	LANL sample number	R	####-##-#### (0121-95-0501)	Sample number assigned by LANL. Note: the container number appears on the sample label as a 2 digit number following the LANL sample ID, it is NOT part of the sample number. For actual samples (SAMPLE or DUP) or derivatives of actual samples (MS or MSD) : Enter the LANL sample number exactly as it appears on the LANL Service Agreement. For laboratory QA/QC samples (e.g, BLANK, ~~MS, MSD,~~ BS, BSD, LCS): leave this field blank. For dilution or re-injection runs: Enter the same LANL sample as the original sample.
B003	LANL container number	R	A10	Number assigned by LANL which uniquely identifies a container which is part of a sample. The container number is generally a two digit number. For actual samples (SAMPLE or DUP) or derivatives of actual samples (MS or MSD) : Enter in exactly as it appears on the LANL Service Agreement. If analysis requires more than a single container, then the LANL container number field should contain a comma delimited list of containers - e.g., 01,03,04 For laboratory QA/QC samples (~~MS, MSD,~~ BLANK, BS, BSD, and LCS): leave this field blank. For dilution or re-injection runs: LANL container number will be the same as for the original sample.
B004	laboratory sample number	R	A25	Number assigned to sample (cut) by the contract laboratory.

B005	laboratory batch reference	R	A20	Batch number in which sample was analyzed. Number should be sufficient to group samples with related laboratory QA/QC samples.
B006	sample quantity	-		
B007	date sampled	-		
B008	matrix	R	A15 (see figure 3)	Matrix of the sample. For actual samples (SAMPLE or DUP) or for laboratory QA/QC samples based on an actual sample (MS, MSD) : choose from one of the possible matrix values listed in figure 3. For blanks (BLANK, BS, or BSD) or laboratory control spikes (LCS): enter a laboratory specific matrix, or choose from the list presented in figure 3.
B009	sample type	R	A10 (see figure 4)	Indicates the type of sample. Choose from the values listed in figure 4.
B010	analytical method code	R	A20	LANL ordering code as specified in the LANL Service Agreement. Figure 5 contains a listing of current ordering codes used by LANL.
B011	reporting units	R	A15 (see figure 6)	Unit of measure used to express the analytic results in this column of the EDD. Figure 6 provides a listing of the mandatory reporting units for each type of analysis. This field should contain only standard characters - i.e., please report in UG/L rather than µG/L.
B012	instrument id	-		
B013	software	-		

Figure 2 - Definitions for Section B

Figure 3 provides a listing of the possible values and associated descriptions for the matrix field. You must use one of these codes for LANL samples, or QA/QC samples based on a LANL sample (e.g., MS, MSD, or DUP). You may use your own lab specific matrix for other QA/QC samples such as BLANK, BS, BSD, or LCS.

Matrix	Description of Matrix
AIR	Sample matrix is air
FILTER	Sample matrix is a filter
MISC	Sample matrix does not fit into any of the other listed categories.
OIL	Sample matrix is oil or primarily oil
SLUDGE	Sample matrix is sludge (contains a significant percentage of both water and soil)
SOIL	Sample matrix is soil
WATER	Sample matrix is a liquid or water
<lab specified>	If the Sample is a laboratory QA/QC sample which is not directly derived from a LANL sample (e.g., BLANK, BS, BSD, or LCS), then you may enter a laboratory specific matrix such as sodium sulfate.

Figure 3 - Valid Matrix Codes

Figure 4 provides a listing of the possible values and associated descriptions for the sample type code field. Contact John Miglio at LANL before you use any other codes.

Sample Type Code	Description of Code
SAMPLE	LANL sample analyzed for specified results
BLANK	Laboratory blank sample
DUP	Laboratory duplicate analysis of a sample (also called replicate)
BS	Blank spike sample (organic analyses)
BSD	Blank spike duplicate sample
MS	Matrix spike sample (organic and rad analyses)
MSD	Matrix spike duplicate sample
LCS	Laboratory Control Sample
SPIKE	Spike sample (inorganic analyses)

Figure 4 - Valid Sample Type Codes

Figure 5 provides a listing of the possible values and associated descriptions for the analytical method code field. Contact John Miglio before you use any other codes.

Analytical Method Code	Description
AM241	Americium-241
GROSSAB	Gross alpha and beta
GROSSG	Gross gamma
GSCAN	Gamma Spec Isotopes
H2O	Moisture Content
H3	Tritium
HENC	Nitrocellulose
HENG	Nitroguandidine
HENGPETN	Nitroglycerine, PETN
HETET	Tetrazene
HEXP	High Explosives 8330 Analytes
HG	Mercury
ICPMS	ICPMS metals
ISOPU	Plutonium-238, 239+40
ISORA	Radium-226, 228
ISOTH	Thorium-228, 230, 232
ISOU	Uranium-234, 235+236, 238
METTAL	Target analyte metals
METTALCN	Target analyte metals with cyanide
METTCLP	TCLP metals
NATTH	Natural Thorium
NATU	Natural Uranium
NP237	Neptunium-237
PB210	Lead-210
PCB	PCBs
PEST	Pesticides
PESTPCB	Pesticides and PCBs
RA226	Radium-226
RA228	Radium-228
SEMI	Semivolatile Organics with Tics
SEMIN	Semivolatile Organics without Tics
SR90	Strontium-90
TCN	Total Cyanide
TH234	Thorium-234
VOAGCMS	Volatile Organics by GC/MS with TICs
VOAGCMSN	Volatile Organics by GC/MS without TICs

Figure 5 - Valid Analytical Method Codes

Figure 6 provides a listing of the mandatory units of measure which should be used with the associated matrix and analytical method code fields. Contact John Miglio at LANL before you use any other units of measure.

Analytical Method Code	Mandatory Reporting Units WATER	SOIL
AM241	PCI/L	PCI/G
GROSSAB	PCI/L	PCI/G
GROSSG	PCI/L	PCI/G
GSCAN	PCI/L	PCI/G
H2O	%	%
H3	PCI/L	PCI/L
HENC	UG/L	MG/KG
HENG	UG/L	MG/KG
HENGPETN	UG/L	MG/KG
HETET	UG/L	MG/KG
HEXP	UG/L	MG/KG
HG	UG/L	MG/KG
ISOPU	PCI/L	PCI/G
ISOTH	PCI/L	PCI/G
ISOU	PCI/L	PCI/G
METTAL	UG/L	MG/KG
NATU	UG/L	MG/KG
PB210	PCI/L	PCI/G
PESTPCB	UG/L	UG/KG
RA226	PCI/L	PCI/G
RA228	PCI/L	PCI/G
SEMIGCMS	UG/L	UG/KG
SR90	PCI/L	PCI/G
TCN	UG/L	MG/KG
VOAGCMS	UG/L	UG/KG

Figure 6 - Mandatory Units

4.3   Section C - Analysis Header

Section C contains the information which is specific to an individual analysis. As such, the contents of this section vary greatly depending on the type of analysis being done. Please refer to the individual EDD sheets in appendix B to determine whether the fields listed in figure7 are required, optional, or not reported for a particular analysis.

During the last design review, a number of fields were deleted. These fields are still contained on the individual EDD. Only those fields in section C which are required or optional on one or more EDD sheets are included in figure 7.

The various EDD sheets were created by a variety of different individuals. Many of the EDD sheets use different labels for the same type of information. For each distinct data field names, their format and a brief description are shown in figure 7.

Label	Format	Description
date of count start	DD-MON-YY	Date when the count was started
time of count start	HH:MM (24 hour clock)	Time when count was started
date of count	DD-MON-YY	Date when the count was started
date acquisition start	DD-MON-YY	Date when the count was started.
time of acquisition start	HH:MM (24 hour clock)	Time when the count was started.
analysis procedure	A30	Reference to the procedure which was used during sample analysis. For rad analyses, this field should contain a reference to the laboratory specific standard operating procedure (SOP) used. For non-rad analyses, this field should contain a reference to the EPA method number.
date of analysis	DD-MON-YY	Date when the analysis (measurement) took place
date of analysis col 1	DD-MON-YY	Same as 'date of analysis' field but used for the first column of a dual column analysis.
date of analysis col 2	DD-MON-YY	Same as 'date of analysis' field but used for the second column of a dual column analysis.
time of analysis	HH:MM (24 hour clock)	Time when the analysis (measurement) began.
time of analysis col 1	HH:MM (24 hour clock)	Same as 'time of analysis' field but used for the first column of a dual column analysis.
time of analysis col 2	HH:MM (24 hour clock)	Same as 'time of analysis' field but used for the second column of a dual column analysis.
dilution factor	###	Dilution factor used to obtain sample results. Should be reported as a whole number without any units. For example, a value of 10 would indicate that the sample has been diluted by a factor of 10.
Florisil cleanup (y/n)	Y or N	'Y' if Florisil cleanup was done. 'N' if it was not done.
GPC Cleanup (y/n)	Y or N	'Y' if gel permeation cleanup was done. 'N' if it was not done.

net mass	number	Net mass of the sample counted in grams
percent moisture	number	The percent moisture in the sample. Should be reported as a percent (i.e., 85.3 rather than 0.853). Do not include a unit of measure (i.e., '%') in this field.
percent solids	number	This field is improperly encoded. It should contain the percent moisture instead. Should be reported as a percent (i.e., 85.3 rather than 0.853). Do not include a unit of measure in this field.
pH	number	The pH of the sample as it is received (before any sample preparation). This field should be reported only if the sample matrix is WATER.
date of preparation	DD-MON-YY	Date when sample was prepared (e.g., extracted, digested, aliquoted, etc.)
date of sample extraction	DD-MON-YY	Date when sample was extracted (see date of preparation).
sample prep procedure	A30	Reference to the procedure which was used during sample preparation. For rad analyses, this field should contain a reference to the laboratory specific standard operating procedure (SOP) used. For non-rad analyses, this field should contain a reference to the EPA method number (e.g., SW 8330)
sample geometry	A16	Geometry for sample count.
sample preservation	Y or N	'Y' if a water sample is acid preserved or if a soil sample is cooled. 'N' otherwise.
Sulfur cleanup (y/n)	Y or N	'Y' if sulfur cleanup was done. 'N' if it was not done.

Figure 7 - Definitions for Section C

4.4   Section E - Analytes

Section E contains the information which is specific to an individual analyte. Virtually all EDD sheets have their own encoding for this section. Please refer to the individual EDD sheets in appendix B to determine whether the fields listed in figure 8 are required, optional, or not reported for a particular analysis.

During the last design review, a number of fields were deleted. These fields are still contained on the individual EDD. Only those fields in section E which are required or optional on one or more EDD sheets are included in figure 8.

The data field names, their format and a brief description are shown in figure 8.

Label	Format	Description
analyte	N/A	Tag and label fields are required, but no data need be entered in individual columns.
technique code	A (figure 9)	Laboratory code indicating method used for analysis. see figure 9 for a listing of valid technique codes.
concentration	number	Sample results.
concentration col 1	number	Sample results for the first column of a dual column method.
concentration col 2	number	Sample results for the second column of a dual column method.
sample activity	number	Sample results.
reported activity	number	Reported activity for the sampled analyte.
~~LCS or MS recovery~~	~~number~~	~~Percent recovery for a LCS or MS sample as a percent (e.g., 85.3 - not 0.85).~~ ~~The unit of measure is assumed to be '%' and so a unit of measure should NOT be included in this field.~~ ~~See section 5.2 for a discussion on how LCS and MS are reported.~~
lab qualifier	A8	Laboratory qualifier associated with the measurement (i.e., sample activity concentration or reported activity)
lab qualifier col 1	A8	Laboratory qualifier associated with the measurement for the first column of a dual column method.
lab qualifier col 2	A8	Laboratory qualifier associated with the measurement for the second column of a dual column method.
1 SD uncertainty	number	One standard deviation of uncertainty for reported activity.
MDA	number	Minimum detectable activity for the specified measurement.
MDC	number	Minimum detectable concentration (NATU only)

Figure 8 - Definitions for Section E

Note: Section E data fields designated on the individual EDDs as being either (R)equired or (O)ptional only need to be reported if you are data concerning that analyte to LANL. For any given analyte that you report, you must include all of the tags for that particular analyte (e.g., the analyte name, concentration, qualifier, etc.) Alternately, you may choose to include all tags in section E and leave the data fields for the analytes you are NOT reporting blank.

Figure 9 provides a listing of the valid technique codes which should be used where the field is marked optional or required. Contact John Miglio at LANL before you use any other technique codes.

Technique Code	Description of Code
P	ICPES
A	Flame AA
F	Graphite Furnace AA
CV	Manual Cold Vapor AA (Mercury)
AV	Automated Cold Vapor AA (Mercury)
AS	Semi-Automated Spectrophotometric (Cyanide)
C	Manual Spectrophotometric (Cyanide)
T	Titrimetric (Cyanide)

Figure 9 - Valid Technique Codes

4.5 Section F - Carriers

Section F contains the information which is specific to an individual carrier. All EDD sheets with carriers use their own encoding. Please refer to the individual EDD sheets to determine whether these fields are optional, required or not used for each type of analysis.

The data field names, their format and a brief description are shown in figure 10.

Label	Format	Description
carrier	N/A	Tag and label fields are required, but no data need be entered in individual columns.
recovery	number * number optionally followed by an asterisk.	Recovery of the carrier specified as a percent (e.g., 85.3 - not 0.853). The unit of measure is assumed to be '%' and so a unit of measure should NOT be included in this field. If the recovery of the carrier is out of control, append an asterisk ('*') to the recovery number (e.g., 285*).

Figure 10 - Definitions for Section F

4.6 Section G - Tracers

Section G contains the information which is specific to an individual tracers. All EDD sheets with tracers use their own encoding. Please refer to the individual EDD sheets to determine whether these fields are optional, required or not used for each type of analysis.

During the last design review, a number of fields were deleted. These fields are still contained on the individual EDD. Only those fields in section G which are required or optional on one or more EDD sheets are included in figure 11.

The data field names, their format and a brief description are shown in figure 11.

Label	Format	Description
tracer	N/A	Tag and label fields are required, but no data need be entered in individual columns.
percent recovered	number * number optionally followed by an asterisk.	Recovery of the tracer specified as a percent (e.g., 85.3 - not 0.853). The unit of measure is assumed to be '%' and so a unit of measure should NOT be included in this field. If the percent recovered is out of control, append an asterisk ('*') to the percent recovered (e.g., 285*)

Figure 11 - Definitions for Section G

4.7   Section H - Surrogates

Section H contains the information which is specific to an individual surrogates. All EDD sheets with surrogates use their own encoding. Please refer to the individual EDD sheets to determine whether these fields are optional, required or not used for each type of analysis.

During the last design review, a number of fields were deleted. These fields are still contained on the individual EDD. Only those fields in section H which are required or optional on one or more EDD sheets are included in figure 12.

The data field names, their format and a brief description are shown in figure 12 below.

Label	Format	Description
surrogate	N/A	Tag and label fields are required, but no data need be entered in individual columns.
percent recovered	###	Recovery of the surrogate specified as a percent (e.g., 85 - not 0.85). A unit of measure or qualifier should NOT be included in this field.
recovered col 1	###	Percent of surrogate compound recovered on the 1st column of a dual column method. Result should be reported as a percent (e.g., 85 - not 0.85) and should not include any unit of measure or qualifier.
recovered col 2	###	same definition as 'recovered col 1' but for 2nd column results
~~concentration col 1~~	~~###~~	~~This field is inappropriately named and was previously incorrectly defined. It should contain the percent recovery for the surrogate run on the 1st column of a dual column method. See 'percent recovered'.~~
~~concentration col 2~~	~~###~~	~~same definition as 'concentration col 1' but for 2nd column results.~~
lab qualifier	A8	Laboratory qualifier associated with the percent recovered
lab qualifier col 1	A8	Laboratory qualifier associated with the percent recovered on the 1st column of a dual column method.
lab qualifier col 2	A8	Laboratory qualifier associated with the percent recovered on the 2nd column of a dual column method.

Figure 12 - Definitions for Section H

Note: Section H data fields designated on the individual EDDs as being either (R)equired or (O)ptional only need to be reported if you are data concerning that surrogate to LANL. For any given surrogate that you report, you must include all of the tags for that particular

surrogate (e.g., the analyte name, recovery, qualifier, etc.) Alternately, you may choose to include all tags in section H and leave the data fields for the surrogates you are NOT reporting blank.

4.8   Section I - Tentatively Identified Compounds

Section I contains the information which is specific to tentatively identified compounds (TIC). All EDD sheets with TICs use their own encoding. Please refer to the individual EDD sheets to determine whether these fields are optional, required or not used for each type of analysis.

The data field names, their format and a brief description are shown in figure 13.

Label	Format	Description
name	A128	Name of the tentatively identified compound as determined by the contract laboratory.
sample results		Amount of the TIC detected.
lab qualifier	A8	Laboratory qualifier associated with the TIC's sample results.
retention time	A16	Retention time for the TIC

Figure 13 - Definitions for Section I

5.0   Clarification on Specific Data

Several types of data being reported on the EDD sheets appear to be problematic in that there is a wide variety of ways in which the data is being reported.

5.1   Surrogates, Carriers, and Tracers

The majority of EDD sheets have surrogates, carriers or tracers. These results should be reported in the same column in the EDD as the associated sample on which they were run. Please follow these rules when reporting this data :

- All surrogates, carriers, and tracers MUST be reported as percent recovered (although the actual field name may vary). The changes to the EDD remove all of the fields which previously stored the amount added and amount recovered.
- The order of the surrogates and their names are important. Do not change the order in which surrogates are reported, nor their tags or names. If you wish to use a surrogate which is not on the appropriate EDD, contact John Miglio.
- Report surrogate, carrier and tracer data only in sections H, F and G respectively. Do not place this data in the comments section or encode it in the analyte's section (section E).
- EDD sheets (HENC,HENG,HENGPETN, HETATB, HETET, and HEXP) which previously asked for concentrations to be reported in the surrogate sections have been corrected. They now indicate that you are to provide the percent recovery for the surrogate.

5.2   Laboratory QA/QC Samples

Laboratory QA/QC samples have caused quite a bit of confusion. Fields such as 'LCS or MS Recovery' on some EDD sheets make it difficult to determine how this information is to be encoded. Please keep the following points in mind when reporting this type of data:

- Each laboratory sample in the EDD should be in its own column. Thus you should report DUP, BLANK, BS, BSD, MS, MSD, and LCS samples in their own columns. Data for these results should NOT be combined with regular samples.
- Most of the rad EDD sheets contain a field for 'LCS or MS Recovery', unfortunately there is no corresponding field in the non-rad EDD sheets. Nor are their fields designed to handle the other laboratory QA/QC sample types. For uniformity, do not use the 'LCS or MS Recovery' fields. Instead report the data in the same fields as you would report normal sample results. Make sure that you are reporting the appropriate type of results and that you fill in the appropriate unit of measure in the reporting units field (B011). For example, if the sample being analyzed is a MS, then the results should be reported as the percent recovered (like all percentages, please report as 93 rather than 0.93) and the reporting units field would be '%'. If the sample was a BLANK, then the unit of measure would be a unit appropriate to the matrix (e.g., MG/KG or UG/L) and the sample result would be the amount of the compound detected in the blank.

5.3   Dual Column Methods

Some EDD sheets, such as pesticides and explosives, are designed to accept dual column results. In many of these analyses, the second column results will not be run unless a 'hit' is detected in the first column results. If available, second column data should be reported in the appropriate fields, otherwise these fields should be left blank.

In general, the fields associated with second column results are marked as O (optional) in both section 4 and in the appropriate EDD sheets. This indicates that there may or may not be a value stored in these fields (the first column result are always required.) However, if the analysis method requires you to run a second column (for example you had a hit on the first column), then you must consider the second column fields as **required** fields.

5.3   Adding/Changing Analytes

The tags associated with the analytes appearing in section E are critical to our ability to correctly extract the data. Do NOT change the encoding (tag, description, or analyte name) of this data. If you need to report data on a compound which is not defined on the EDD, please contact John Miglio for instructions. LANL may decide to add a new set of tags for that particular compound to the EDD or to ask you to report the data in some other manner (possibly by hard copy only). If LANL adds a new set of tags, then that information will be distributed to all contract laboratories.

5.4   Reporting Values Below Stated Levels

Note that the EDD sheets use different methods to report limits of quantitation, detection or other agreed upon reporting limits. The rad EDD sheets have included a field to be used to report either the MDA or MDC.   When reporting rad data, the appropriate field should always be filled in.

However, there is no corresponding field in the non-rad EDD sheets. Some of the EDD sheets, such as VOAGCMS, specify that the concentration field should contain either the sample result or the estimated quantitation limit if the compound was not detected. In the latter case, be sure to enter the appropriate qualifier in the lab qualifier field. Other EDD sheets, such as pesticides, indicate that the concentration field should merely contain the sample result. No mention is made of how to handle results below the reporting limits.

The best solution would be to add a field, similar in function to the MDA field, for non-rad results. Unfortunately, this would results in a significant change to a large number of EDD sheets. Instead, for non-rad data, if the compound or analyte is not detected at levels at or above the limits (EQL, detection, or agreed upon reporting limit), then the limit should be reported in the sample results field (AKA, concentration) and the appropriate qualifier should be entered into the lab qualifier field.

5.5 File Formats & Submitting the EDD

EDD data may be submitted to LANL as an ASCII file and delivered either electronically (email or ftp) or on a floppy disk. When creating the ASCII file, please generate a tab delimited file (the fields are separated by a tab). Please do not submit export files in either comma delimited or fixed width form. In addition, files which do not use the most recent EDD structure will not be accepted.

6.0 Contacts & Further Information

For questions concerning analytic methods, analytes to be reported or any contractual issues, please contact:

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For issues concerning the encoding of the EDD (except where otherwise noted), please contact FIMAD:

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